4-Nitrosodiphenylamine 156-10-5 | DTXSID1021031

Model Performance

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Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 325 °C

Global applicability domain: Inside

Local applicability domain index: 3.54e-01

Confidence level: 5.62e-01

Nearest Neighbors from the Training Set

Image not found

4-Nitrosodiphenylamine

Measured: 292 Predicted: 325

Image not found

N-Phenyl-1,4-benzenediamine

Measured: 354 Predicted: 363

Image not found

1,2-Benzenediamine,N-phenyl-

Measured: 313 Predicted: 363

Image not found

4,4'-Oxydianiline Measured: 350 Predicted: 363

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2,4'-Biphenyldiamine Measured: 363 Predicted: 367